

Optical Conductivity of the Two-Dimensional Hubbard Model

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Charge dynamics of the two-dimensional Hubbard model is investigated. Lancz s-diagonalization results for the optical conductivity and the Drude weight of this model are presented. Near the Mott transition, large incoherence below the upper-Hubbard band is obtained together with a remarkably suppressed Drude weight in two dimensions while the clearly coherent character is shown in one dimension. The two-dimensional results are consistent with previous results from quantum Monte Carlo calculations indicating that the Mott transition in this two-dimensional model belongs to the universality class characterized by the dynamical exponent of $z = 4$.

KEYWORDS: two-dimensional Hubbard model, Mott transition, optical conductivity, Drude weight, incoherence, exact diagonalization, dynamical exponent

Physics of metal-insulator transitions is one of the major issues in current condensed-matter physics from both experimental and theoretical viewpoints.¹⁾ The Hubbard model is one of the simplest models which can describe the metal-insulator transition. This model shows a Mott transition originating in strong correlation between electrons. Unfortunately, properties of this model in two and three dimensions are not completely understood.

According to the scaling hypothesis for the Mott transition,²⁾ the Drude weight and the compressibility have the critical dependence on the doping concentration δ as $D \propto \delta^{1+(z-2)/d}$ and $\kappa \propto \delta^{1-z/d}$, respectively, where z denotes the dynamical exponent and d represents the spatial dimension. The transition is characterized by z . The value of z may depend on systems and the scaling theory (ST) itself does not determine it. To fix the value of z , one has to estimate it explicitly, for example, using numerical results. Dagotto *et al.* reported $D \propto \delta$ for the two-dimensional (2D) Hubbard model.³⁾ If one employs the ST, $D \propto \delta$ suggests $z = 2$, which is in the same universality class as the band metal-insulator transition. From the quantum Monte Carlo (QMC) calculations,⁴⁾ on the other hand, the chemical potential μ is scaled by δ^2 . This leads to $\kappa \propto 1/\delta$ and $z = 4$. Another QMC calculation for the chemical-potential dependence of the localization length, ξ_l , shows $\xi_l = |\mu - \mu_c|^{-\nu}$ with $\nu = \frac{1}{4}$,⁵⁾ which also suggests $z = 4$. Thus, if one is based on the ST, a discrepancy remains between these two QMC results and the above result by Dagotto *et al.*, which could pose a suspicion on the validity of the ST.

Quite recently, it was reported that D in the 2D t - J model has a very small value near the Mott transition, which strongly indicates $z = 4$.⁶⁾ The critical behavior of $\kappa \propto 1/\delta$ in this model was also reported.⁷⁾ Since the t - J model is obtained in the strong-coupling limit of the Hubbard one in small J/t , it is widely believed that these models show the same critical behavior at least at realistic values of J/t . To have further insight on this issue, in our present analyses, we treat the finite-size (FS) effect more carefully than in the literature and reexamine the optical conductivity of the 2D Hubbard model.

We study a model given by $\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$, where the creation(annihilation) of an electron at site i with spin σ is denoted by $c_{i\sigma}^\dagger (c_{i\sigma})$ with the number operator $n_{i\sigma}$. Here, we treat only the nearest-neighbor hopping with amplitude $t=1$. The doping concentration is given by $\delta = 1 - \frac{N_e}{N_s}$, where N_e and N_s denote the number of electrons and sites, respectively. We choose a boundary condition (BC) among periodic, anti-periodic and mixed⁸⁾ ones so that the ground-state energy becomes as low as possible as it should be. In fact, with this procedure, negative and unphysical values of D obtained in Ref. 3 near half filling do not appear because D is the curvature of the flux dependent energy at the true ground state. The FS effect in this procedure is expected to be smaller than the fixed BC. Actually, when one considers the sum of squared deviations from the thermodynamic limit in D of 4×4 -site system with even N_e at $U=0$, the sum for the optimized BC is ~ 0.0021 , smaller than ~ 0.0032 for the BC fixed to be periodic.

We use exact diagonalization of an FS cluster of 4×4 sites based on Lancz s algorithm and continued-fraction-expansion method.⁹⁾ Hilbert space of this cluster has a huge dimension of order of 10^8 . To treat the dimension, we carry out the parallel processing on supercomputers with a distributed-memory system.

We here calculate the optical conductivity defined as $\sigma(\omega) = [\sigma_x(\omega) + \sigma_y(\omega)]/2$ with $\sigma_\alpha(\omega)$ given by $2\pi e^2 D_\alpha \delta(\omega) + \frac{\pi e^2}{N} \sum_{n \neq 0} \frac{|\langle n | j_\alpha | 0 \rangle|^2}{E_n - E_0} \delta(\omega - E_n + E_0)$. Here D_α is the Drude weight along α -direction ($\alpha=x, y$) and j_α is a current operator along the α -direction defined as $j_\alpha = -i \sum_{i, \sigma} t (c_{i\sigma}^\dagger c_{i+\delta_\alpha, \sigma} - c_{i+\delta_\alpha, \sigma}^\dagger c_{i\sigma})$, where δ_α is the unit vector along the α -direction. $|n\rangle$ denotes an eigenstate with the energy eigenvalue of E_n . The ground state is represented by $n = 0$. The averaging operation is performed to handle the anisotropic results due to the mixed BC and to reduce the FS correction. The Drude weight can be obtained from the combination of $\sigma(\omega)$ and the sum rule of $\int_0^\infty \sigma(\omega) d\omega = \pi e^2 K$, where $4K$ denotes the kinetic energy per site. Hereafter we will call K the total weight. When U is large enough, we also calculate an effective carrier density defined as $N_{\text{eff}} = \frac{1}{\pi e^2} \int_0^{\omega_c} \sigma(\omega) d\omega$, where ω_c is a frequency just below the upper-Hubbard (UH) band. If U is small, weight transfer to the UH band and the one within the lower-Hubbard band merge and N_{eff} is not well defined. To find ω_c definitely, we take a large value of $U/t = 16$. Note that, in the t - J limit of $U \rightarrow \infty$, N_{eff} is equal to K . Besides, one can expect that the large value of U would reduce the FS effect. In this work, we make a further procedure to reduce the FS effect. The procedure is to multiply

a correction factor defined by $r = K_\infty/K_{N_s}$, where K_∞ and K_{N_s} are the total weights for $U=0$ in the thermodynamic limit and of the N_s -site system, respectively. Hereafter, all the quantities obtained after this procedure are labeled with suffix c, for example, D^c . To check the validity of our calculations, we show results for the 1D Hubbard chain with $U/t = 16$ in the inset of Fig. 1. It is seen that our Drude weight excellently agrees with the Bethe-ansatz result in the thermodynamic limit.¹⁰⁾ Here one can also see the coherent feature, namely, $N_{\text{eff}}^c - D^c \ll N_{\text{eff}}^c$ in the whole region of δ .

Now, we present the results for the 2D Hubbard model with $U/t = 16$ in Fig. 1. At half filling, the Drude weight is positive and finite but very small. This small and finite value comes from the FS effect and is expected to converge to zero if systems become larger. Actually, we have obtained $D^c \sim 0.028$ for $\sqrt{10} \times \sqrt{10}$ sites for the same U at half filling whereas $D^c \sim 0.008$ for 4×4 sites, which shows a rapid convergence to zero. In the dilute-electron-density region ($\delta \sim 1$), the interaction effect is small and the three quantities are close to the $U=0$ case. At larger electron density, the interaction works to prevent the electron motion and the three quantities decrease. In the whole region of δ , N_{eff} exhibits a smooth and convex curve. In contrast with the results in Ref. 3, compared to N_{eff} , D shows a concave shape below $\delta = 0.25$ as shown in the data point closest to the Mott transition while an overall convex behavior for higher δ . This makes a quite asymmetric curve of D between $\delta < 0.5$ and $\delta > 0.5$ under reflection with respect to $\delta=0.5$. The concave shape for small δ suggests $z > 2$. Although the number of data point at small δ is not sufficient to draw a definite conclusion on the exponent, the present result obtained after carefully reducing the FS effect supports that, as $\delta \rightarrow 0$, D vanishes faster than linear δ -dependence, and does not contradict $D \propto \delta^2$. The exponent deduced from $D \propto \delta^2$ is consistent with the ST characterized by $z = 4$, and agrees with other results from the QMC method.^{4,5)}

Let us discuss the frequency dependence of the optical conductivity for $U/t=16$ shown in Fig. 2(a)-(d). At half filling, only the excitations to the UH band are seen in Fig. 2(a). Upon increasing δ , weights are transferred to the region below the Hubbard gap. In Fig. 2(b), one can see the large incoherent part below the UH band. The mid-gap incoherence has a larger weight on the lower-frequency side. As the frequency is increased, the height of the incoherence gradually decreases after the highest peak at about $\omega/t \sim 2$. It is tempting to relate this structure to the shape of the $1/\omega$ tail seen in the experiment of high- T_c compound, although the incoherent response in the small frequency side $\omega/t < 2$ clearly suffers from the FS effect. A similar behavior is seen in the study of the 2D t - J model.^{11,12,13)} Note that the data which Dagotto *et al.* reported in Ref. 3 did not show such structure because the mid-gap incoherence itself is too small at the same $\delta=0.125$. Note also that the present calculations show that the incoherent peak gradually loses its weight with increasing δ while the long-tail structure survives.

In summary, we have investigated the charge dynamics of the 2D Hubbard model. Lanczöš

diagonalization results under the careful treatment of the boundary condition have been presented. Near the metal-insulator transition, the optical conductivity has the large incoherence in the mid-gap region. At that doping concentration, the Drude weight is clearly suppressed, which supports the $z = 4$ universality class of the Mott transition.

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Fig. 1. Drude weight, effective carrier density and total weight of the 2D Hubbard model when $U/t = 16$. Inset shows the 1D results for 10 and 12 sites for $U/t = 16$ together with the Bethe-ansatz result in the thermodynamic limit¹⁰⁾ (solid curve) for comparison.

Fig. 2. Incoherent part of $\sigma(\omega)$ for (a) $\delta=0$ (anti-periodic BC), (b) $\delta=0.125$ (mixed), (c) $\delta=0.25$ (mixed), (d) $\delta=0.375$ (periodic). Delta functions in the peaks are broadened with width of $\epsilon=0.05$.



